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TABLE OF TRIM DISCRETE QUADRATURE PARAMETERS FOR THIN BINARY SLAB CELLS

by

David Meneghetti

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TABLE OF TRIM DISCRETE QUADRATURE PARAMETERS
FOR THIN BINARY SLAB CELLS

by

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Reactor Engineering Division

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**TABLE OF TRIM DISCRETE QUADRATURE PARAMETERS
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ABSTRACT

Discrete quadrature weights and angles for use in discrete ordinate methods of solutions for thin cells are tabulated for a series of regional cell thicknesses of applicability. Parameters are given for 4, 6, 8, 10, and 12 angle approximations. The quadrature assignments are based upon a simplified integral transport solution to the spatial average of the angular distribution of uncollided flux, assuming flat sources. The quadrature assignments are designated TRIM, for thin-region integral method, and are most useful with thin cells having either or both regions very thin in mean-free-path units. The IBM-704 Fortran program used to compute the parameters is described.

I. INTRODUCTION

It is generally necessary to use a high-order, discrete-ordinate approximation, i.e., many discrete angles, in order to obtain sufficiently accurate flux solutions for thin-slab cells. This is, for example, observed in the calculation of heterogeneity effects in fast critical assemblies using the discrete S_N method (DSN).⁽¹⁾ Analysis of the problem and comparative calculations using single and double Gaussian quadratures have also been reported.⁽²⁾ Two additional quadratures have subsequently been suggested.⁽³⁾ One is based upon a modification of the single Gaussian quadrature. The other is based upon the angular distribution of uncollided flux as obtained by integral transport theory. These are designated MSG, for modified single Gaussian; and TRIM, for thin-region integral method.

Criteria for determining a priori the suitability of double Gaussian (DG), MSG, or TRIM quadratures were also reported.⁽³⁾ Quadrature choice depends upon the regional thicknesses in mean-free-path units and upon the number of discrete angles to be employed. Whenever feasible, DG or MSG quadratures are preferred, as the parameters are already available for the former and easily obtainable for the latter by transformation of available single Gaussian parameters. The transformations are

$$\left| \mu_\lambda^{\text{MSG}} \right| = 1 - \left| \mu_\lambda^{\text{SG}} \right| \quad \text{and} \quad R_\lambda^{\text{MSG}} = R_\lambda^{\text{SG}}$$

for the discrete angles and weights, respectively. For thin cells the MSG is more favorable than DG, because the discrete angles are distributed with relatively greater density in the region of small $|\mu|$ which is the region of predominant anisotropy of the flux. It has been found for a binary cell having regional thicknesses A and B, in mean-free-path units, DG or MSG is suitable if there is at least one discrete angle

$$|\mu_{\min}| \gtrsim \frac{1}{2} \left(\frac{AB}{A+B} \right)$$

among the $N/2$ values of $|\mu_\lambda|$ for that quadrature.⁽³⁾ A TRIM quadrature is otherwise suggested.

TRIM parameters must be specifically chosen for the particular cell. In order to have a set of TRIM parameters readily available, the present table has been prepared.

II. CONSTRUCTION OF TABLE

The concept, use, and accuracy of TRIM quadratures for thin binary cells have been previously described.⁽³⁾ The present table is based upon the nonisotropic average angular distribution function⁽³⁾

$$g(|\mu|) \equiv (1 - e^{-\alpha}) - |\mu| \left(1 - e^{-\alpha/|\mu|} \right) \quad (1)$$

and its integral from $\mu = 0$ to $|\mu|$:

$$y(|\mu|) \equiv |\mu| (1 - e^{-\alpha}) - \frac{\alpha}{2} |\mu| e^{-\alpha/|\mu|} - \frac{|\mu|^2}{2} \left(1 - e^{-\alpha/|\mu|} \right) + \frac{\alpha^2}{2} E_1(x). \quad (2)$$

$$\alpha = \frac{AB}{A+B} \text{ and } E_1(x) = \int_x^\infty \frac{e^{-v}}{v} dv \text{ with } x = \frac{\alpha}{|\mu|} \quad .$$

The weights R_λ ($\lambda = 1, 2, \dots, N/2$) are assigned to be equal to the intervals $(\Delta\mu)_\lambda \equiv \mu_\lambda - \mu_{\lambda-1}$ which divide $y(1)$ into $N/2$ equal areas, i.e.,

$$\frac{y(\mu_\lambda)}{y(1)} = \frac{\lambda}{N/2}, \quad (3)$$

where N is an even number denoting the total number of discrete angles. The absolute values of the discrete angles, $|\bar{\mu}_\lambda|$, are then obtained from the relation

$$R_\lambda \frac{y(|\bar{\mu}_\lambda|)}{y(1)} = \frac{1}{N/2}. \quad (4)$$

The IBM-704 Fortran program used to carry out the computation of the R_λ and $|\bar{\mu}_\lambda|$ is given in the Appendix.

The α -range of the table is $0.005 \leq \alpha \leq 0.5$ in increments sufficiently small that use of parameters for the listed α -value nearest to $AB/(A+B)$ will generally suffice. The parameters are listed for approximation $N = 4, 6, 8, 10$, and 12.

III. USE OF TABLE

Consider the binary cell having A and B, the total regional thicknesses, in units of total regional mean free paths. If there exists for DG or MSG quadratures in the N-approximation decided upon, a $|\bar{\mu}_{\min}| \lesssim \frac{1}{2} \left(\frac{AB}{A+B} \right)$, then TRIM need not be used.

If TRIM is indicated, choose from among the listed N-approximations, corresponding to the α nearest to $\left(\frac{AB}{A+B} \right)$, an N-approximation which has a minimum of at least one value of

$$|\bar{\mu}_\lambda| \lesssim \frac{1}{2} \left(\frac{AB}{A+B} \right) .$$

APPENDIX

Description and Fortran Listing of IBM-704 Program:

RE-1421 TRIM QUADRATURE CONSTANTS FOR THIN CELLS

Data Input Card 1

Contains the quantities A, ERR, EPS in FORMAT (6E 12.4), where A is the quantity referred to as α in the text; ERR is a convergence-criterion parameter in the $E_m(x)$ subroutine, CALLEONE; and EPS is the convergence criterion on the equalities of Eqs. (3) and (4).

Cards 2, 3, . . . Each contains the integer quantity $N \leq 10$ in FORMAT (15). Here, N is the number of positive angles contained in the quadrature approximation desired. Also, $ERR = 10^{-6}$ and $EPS = 10^{-4}$ have been found suitable for $\alpha \gtrsim 0.005$ and $N \geq 6$. If parameters for smaller α or large N should be required, it may be necessary to assign different ERR and EPS values.

Fortran library tape is to be on tape No. 1.

Overflow in.

Output

On Line. The weights R_i , $i = 1, \dots, N$, are printed for the first N - value. The discrete angles $|\bar{\mu}_i|$, $i = 1, \dots, N$, are next printed, for the same N-value, beginning with a new row. Outputs corresponding to next N-value then follow similarly.

TRIM QUADRATURE PARAMETERS

$ \bar{\mu}_1 $	$ \bar{\mu}_2 $	$ \bar{\mu}_3 $	$ \bar{\mu}_4 $	$ \bar{\mu}_5 $	$ \bar{\mu}_6 $	R_1	R_2	R_3	R_4	R_5	R_6
$\alpha = 0.005$											
0.00815	0.2701	0.3473				0.0261	0.9739	0.9325			
0.00373	0.0304	0.0586	0.4041			0.0098	0.0577	0.0837	0.8901		
0.00240	0.0137	0.0276	0.0879	0.4477		0.0057	0.0205	0.0315	0.1028	0.8511	
0.00177	0.00837	0.0333	0.0992	0.4627	0.1165	0.4827	0.0039	0.0107	0.0164	0.0414	0.1166
0.00141	0.00591	0.0168	0.0437			0.0030	0.0067				0.8159
$\alpha = 0.0075$											
0.0104	0.2843	0.3626				0.0317	0.9683	0.9224			
0.00494	0.0364	0.0677	0.4193			0.0125	0.0651	0.0909	0.8774		
0.00323	0.0172	0.0750	0.4308			0.0074	0.0243	0.0359	0.1092	0.8366	
0.00240	0.0108	0.0333	0.0992	0.4627		0.0052	0.0131	0.0393	0.1138	0.1219	0.8006
0.00191	0.00774	0.0208	0.0514	0.1292		0.4973	0.0040	0.0085	0.0192	0.0458	
$\alpha = 0.01$											
0.0123	0.2952	0.3740				0.0364	0.9636	0.9144			
0.00599	0.0413	0.0560	0.4308			0.0149	0.0707	0.0963	0.8673		
0.00397	0.0201	0.0750	0.4740			0.0090	0.0274	0.0359	0.1092	0.8254	
0.00297	0.0129	0.0381	0.1081	0.1394		0.0064	0.0151	0.0393	0.1138	0.1258	0.7886
0.00236	0.00933	0.0243	0.0577			0.5083	0.0050	0.0099	0.0215	0.0492	
$\alpha = 0.02$											
0.0183	0.3245	0.4044				0.0505	0.9495	0.8916			
0.00954	0.0560	0.0667	0.4607			0.0224	0.0860	0.1099	0.8396		
0.00646	0.0294	0.0958	0.5032			0.0141	0.0364	0.0484	0.1252	0.7950	
0.00489	0.0196	0.0524	0.1333	0.1671		0.0103	0.0211	0.0325	0.0579	0.1348	0.7568
0.00392	0.0145	0.0349	0.0760			0.5366	0.0081	0.0144	0.0280		
$\alpha = 0.03$											
0.0231	0.3437	0.4242				0.0609	0.9391	0.8756			
0.0124	0.0667	0.1105	0.4801			0.0284	0.0960	0.1182	0.8210		
0.00850	0.0365	0.0750	0.5218			0.0182	0.0426	0.0546	0.1317	0.7748	
0.00647	0.0248	0.0630	0.1504	0.1862		0.5544	0.0134	0.0255	0.0325	0.0635	0.1401
0.00523	0.0188	0.0430	0.0892			0.0106	0.0177	0.0229			
$\alpha = 0.04$											
0.0272	0.3585	0.4389				0.0693	0.9307	0.8631			
0.0149	0.0756	0.1222	0.4944			0.0333	0.1036	0.1243	0.8064		
0.0103	0.0424	0.0750	0.5356			0.0217	0.0476	0.0591	0.1364	0.7593	
0.00785	0.0293	0.0715	0.1639	0.2005		0.5677	0.0161	0.0291	0.0360	0.0676	0.1433
0.00635	0.0223	0.0497	0.1000			0.0128	0.0205	0.0369			0.7198
$\alpha = 0.05$											
0.0308	0.3705	0.4510				0.0767	0.9233	0.8526			
0.0171	0.0831	0.1322	0.5060			0.0377	0.1097	0.1291	0.7942		
0.0119	0.0476	0.0879	0.5467			0.0249	0.0518	0.0629	0.1400	0.7463	
0.00911	0.0332	0.0855	0.1753	0.2128		0.5784	0.0186	0.0322	0.0389	0.0708	0.1460
0.00730	0.0255	0.0556	0.1087			0.0148	0.0229				0.7066
$\alpha = 0.06$											
0.0340	0.3807	0.4611				0.0831	0.9169	0.8434			
0.191	0.0897	0.1406	0.5158			0.0417	0.1149	0.1329	0.7840		
0.0133	0.0523	0.0855	0.1849	0.2231		0.5875	0.0277	0.0554	0.0660	0.1428	0.7355
0.0102	0.0368	0.1235	0.2014	0.2408		0.0167	0.0250	0.0414	0.0735	0.1481	0.6953
0.00827	0.0284	0.0608	0.1166			0.0128	0.0229				
$\alpha = 0.07$											
0.0370	0.3897	0.4778				0.0889	0.9111	0.8533			
0.0210	0.0956	0.1552	0.5317			0.0453	0.1194	0.1363	0.7748		
0.0147	0.0565	0.1483	0.5643			0.0303	0.0586	0.0689	0.1453	0.7256	
0.0113	0.0400	0.0913	0.1936	0.2324		0.5953	0.0229	0.0373	0.0436	0.0757	0.1498
0.00910	0.0310	0.0656	0.1235			0.0183	0.0269	0.0436			0.6857
$\alpha = 0.08$											
0.0397	0.3976					0.0942	0.9058	0.8280			
0.0227	0.1010					0.0486	0.1234	0.1392	0.7666		
0.0159	0.0603					0.0328	0.0614	0.0712	0.1473	0.7173	
0.0122	0.0430					0.0247	0.0395	0.0455	0.0778	0.1512	0.6769
0.00996	0.0335					0.0199	0.0287				

TRIM QUADRATURE PARAMETERS (Cont'd.)

$ \bar{\mu}_1 $	$ \bar{\mu}_2 $	$ \bar{\mu}_3 $	$ \bar{\mu}_4 $	$ \bar{\mu}_5 $	$ \bar{\mu}_6 $	R_1	R_2	R_3	R_4	R_5	R_6
$\alpha = 0.09$											
0.0422	0.4048	0.1060	0.4849	0.5385		0.0991	0.9009	0.8213			
0.0243		0.0639	0.1615			0.0517	0.1270				
0.0171		0.0639	0.1015	0.2083	0.5779	0.0350	0.0640	0.1418	0.7592		
0.0131	0.0459		0.1015			0.0265	0.0415	0.0733	0.1489	0.7098	
0.0107	0.0358		0.0737	0.1359	0.2480	0.6080	0.0214	0.0303	0.0473	0.0797	0.1523
$\alpha = 0.10$											
0.0447	0.4113	0.1107	0.4913	0.5446		0.1036	0.8964	0.8152			
0.0258		0.0673	0.1672			0.0546	0.1302				
0.0182		0.0673	0.1060	0.2146	0.5837	0.0372	0.0665	0.1439	0.7524		
0.0140	0.0485		0.1252			0.0282	0.0434	0.0753	0.1505	0.7026	
0.0113	0.0379		0.0776	0.1411	0.2549	0.6138	0.0228	0.0319	0.0490	0.0812	0.1533
$\alpha = 0.15$											
0.0549	0.4378	0.1300	0.5168	0.5689		0.1226	0.8774	0.7901			
0.0323		0.0816	0.1913			0.0670	0.1429				
0.0229		0.0816	0.1252	0.2411	0.6067	0.0463	0.0763	0.1526	0.7248		
0.0176	0.0597		0.1635			0.0355	0.0511	0.0831	0.1562	0.6741	
0.0144	0.0473		0.0933			0.0288	0.0382	0.0555	0.0874	0.1570	0.6331
$\alpha = 0.20$											
0.0631	0.4575	0.1453	0.5356	0.5866		0.1375	0.8625	0.7708			
0.0375		0.2098				0.0769	0.1523				
0.0266	0.0929		0.2250			0.0537	0.0837	0.1587			
0.0207	0.0688		0.1402	0.2613	0.6234	0.0414	0.0572	0.0889	0.1600	0.6525	
0.0168	0.0546		0.1058	0.1808	0.3031	0.6517	0.0337	0.0432	0.0605	0.0918	0.1589
$\alpha = 0.25$											
0.0700	0.4733	0.1578	0.5506	0.6008		0.1498	0.8502	0.7550			
0.0420		0.1024	0.2377			0.0853	0.1597				
0.0299		0.1526	0.2775			0.0599	0.0898	0.1632			
0.0232	0.0764		0.1163			0.0463	0.0621	0.0934	0.1626	0.6356	
0.0189	0.0612		0.1163	0.1950	0.3202	0.6642	0.0378	0.0475	0.0645	0.0952	0.1605
$\alpha = 0.30$											
0.0759	0.4865	0.1687	0.5631	0.6123		0.1603	0.8397	0.7417			
0.0457		0.1106	0.2377			0.0924	0.1659				
0.0327	0.0828		0.1633	0.2911	0.6476	0.0654	0.0950	0.1668	0.6728		
0.0253	0.0665		0.1253	0.2070	0.3343	0.6747	0.0507	0.0663	0.0972	0.1647	0.6211
0.0207						0.0414	0.0510	0.0679	0.0980	0.1614	0.5803
$\alpha = 0.35$											
0.0812	0.4978	0.1779	0.5736	0.6223		0.1696	0.8304	0.7302			
0.0490		0.1181	0.2488			0.0988	0.1710				
0.0349		0.0887	0.1725	0.3028	0.6569	0.0701	0.0995	0.1698	0.6606		
0.0272	0.0714		0.1330	0.2173	0.3464	0.6835	0.0544	0.0701	0.1003	0.1663	0.6089
0.0223						0.0446	0.0542	0.0708	0.1002	0.1621	0.5681
$\alpha = 0.40$											
0.0857	0.5078	0.1864	0.5828	0.6310		0.1776	0.8224	0.7201			
0.0517		0.1242	0.2584			0.1043	0.1756				
0.0372	0.0939		0.1807	0.3133	0.6650	0.0743	0.1033	0.1722	0.6502		
0.0289	0.0754		0.1401	0.2268	0.3571	0.6911	0.0578	0.0734	0.1031	0.1676	0.5981
0.0237						0.0474	0.0569	0.0733	0.1023	0.1627	0.5574
$\alpha = 0.45$											
0.0898	0.5166	0.1939	0.5910	0.6386		0.1849	0.8151	0.7110			
0.0545		0.1299	0.2670			0.1094	0.1796				
0.0391		0.0984	0.1881	0.3229	0.6722	0.0781	0.1068	0.1744	0.6407		
0.0304	0.0794		0.1463	0.2353	0.3667	0.6977	0.0609	0.0763	0.1055	0.1689	0.5884
0.0250						0.0499	0.0594	0.0756	0.1040	0.1632	0.5479
$\alpha = 0.50$											
0.0935	0.5244	0.2006	0.5984	0.6454		0.1915	0.8085	0.7030			
0.0567		0.1352	0.2751			0.1139	0.1831				
0.0408		0.1025	0.1947	0.3312	0.6784	0.0815	0.1100	0.1764	0.6321		
0.0318	0.0761		0.1463	0.2353	0.3753	0.7038	0.0637	0.0789	0.1077	0.1699	0.5798
0.0261	0.0690		0.1521	0.2426		0.0522	0.0617	0.0776	0.1055	0.1637	0.5393


```

C   TRIM QUADRATURE CONSTANTS FOR THIN CELLS
DIMENSIONAMU(10),R(10),UBAR(10)
1 FORMAT(6E12.4)
2 FORMAT(I5)
READ1,A,ERR,EPS
3 READ2,N
PA=EXP(-A)
CALLEONE(A,ESUBM,ERR)
AINTM=0.5*(1.0-PA)-0.5*A*PA+0.5*A*A*ESUBM
L=N-1
4 D020M=1,L
U=0.5
UMIN=0.0
UMAX=1.0
5 XA=A/U
PXA=EXP(-XA)
CALLEONE(XA,ESUBA,ERR)
EM=M
EN=N
YU=-EM/EN+(U*(1.0-PA)-0.5*U*U*(1.0-PXA))
X-0.5*A*U*PXA+0.5*A*A*ESUBA)/AINTM
IF(ABSF(YU)-EPS)11,11,12
11 AMU(M)=U
GOTO20
12 IF(YU)13,14,15
13 UMIN=U
U=(UMIN+UMAX)/2.0
GOTOS
14 STOP
15 UMAX=U
U=(UMAX+UMIN)/2.0
GOTOS
20 CONTINUE
25 FORMAT(1P8E14.5)
AMU(N)=1.0
R(1)=AMU(1)
R(N)=AMU(N)-AMU(L)
IF(L-2)26,21,21
21 D022M=2,L
22 R(M)=AMU(M)-AMU(M-1)
26 PRINT25,(R(I),I=1,N)
UBMIN=0.0
28 D036I=1,N
UBMAX=AMU(I)
29 UB=(UBMIN+UBMAX)/2.0
XB=A/UB
PXB=EXP(-XR)
ZU=-1.0/EN+R(I)*(1.0-PA-UB*(1.0-PXB))/AINTM
IF(ABSF(ZU)-EPS)30,30,31
30 UBAR(I)=UB
UBMIN=AMU(I)
GOT036
31 IF(ZU)34,33,32
32 UMIN=UB
GOTO29
33 STOP
34 UMAX=UB
GOTO29
36 CONTINUE
PRINT25,(UBAR(I),I=1,N)
GOT03
END(0,1,0,0,0)

```


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